Conditions for Efimov Physics for Finite Range Potentials

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We consider a system of three identical bosons near a Feshbach resonance in the universal regime with large scattering length usually described by model independent zero-range potentials. We employ the adiabatic hyperspherical approximation and derive the rigorous large-distance equation for the adiabatic potential for finite-range interactions. The effective range correction to the zero-range approximation must be supplemented by a new term of the same order. The non-adiabatic term can be decisive. Efimov physics is always confined to the range between effective range and scattering length. The analytical results agree with numerical calculations for realistic potentials.

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Introduction. Universal scaling properties in three-body systems arise when the scattering length a is much larger than the range r_0 of the underlying two-body potential [1]. In this regime certain three-body observables are universal in the sense that they are model independent. This is colloquially referred to as Efimov physics [2, 3, 4, 5]. Examples can be found in nuclear systems, small molecules, and particularly in cold atoms where the scattering length can be tuned to desired values using the Feshbach resonance technique.

The universal scaling of Efimov trimers is usually said to exist for rms-sizes between r_0 and a [1, 3, 4, 6]. The effective range R_e from a low-energy phase shift expansion is sometimes used instead of r_0 in this statement [5, 7, 8]. This ambiguity occurs because r_0 and R_e are often of the same order. However, for narrow Feshbach resonances in atomic gases R_e can be much larger than r_0 [9], and the implications for such systems need to be explored.

Zero-range models, in particular in combination with the hyperspherical approximation [4, 7, 10], have been successful in semi-quantitative descriptions of three-body systems in the universal regime. Semi-rigorous finite-range corrections have been attempted by including the higher order terms in the effective range expansion [5, 7] as a step towards the full finite-range calculations as in [8, 11] while maintaining the conceptual and technical simplicity of the zero-range approximation.

The obvious generalization of the zero-range model is to substitute $-1/a$ with $-1/a+(R_e/2)k^2$, where k is the two-body wave-number, in the relevant expressions for the logarithmic derivative of the total wave-function at small separation of the particles. However, in three-body systems neither the two-body wave-number nor the small separation are uniquely defined, and rigorous inclusion of all terms of the given order is non-trivial. The lack of rigor in previous works could have serious implications for applications where finite-range effects are important, such as the stability conditions for condensates in traps, properties of cold atoms in lattices, and generally for Efimov physics. Experimental progress [3] will soon require this increased accuracy near the boundaries of the universal regime.

In this Letter we derive, within the adiabatic hyperspherical approximation [12], the rigorous asymptotic equation for the adiabatic potential, which includes the finite-range correction terms. The equation is suitable for the analytic studies of the finite-range corrections in the three-boson problem. We investigate the finite range corrections to the adiabatic potential and the non-adiabatic term and compare with the zero-range approximation.

Adiabatic eigenvalue equation. We consider three identical bosons of mass m and coordinates $\boldsymbol{r}_i$ interacting via a finite-range two-body potential V, where we assume $V(r_{jk}) = 0$ for $r_{jk} = |\boldsymbol{r}_j - \boldsymbol{r}_k| > r_0$. Only relative s-waves are included. We use the hyperradius $\rho^2 = (r_{12}^2 + r_{13}^2 + r_{23}^2)2\mu/3$ and hyperangles $\tan\alpha_i = (r_{jk}/r_{i,jk})\sqrt{3}/2$, where $r_{i,jk} = |\boldsymbol{r}_i - (\boldsymbol{r}_j + \boldsymbol{r}_k)/2|$ and μ is an arbitrary parameter [12]. In the following we shall use one set of coordinates and omit the index.

The adiabatic hyperspherical approximation treats the hyperradius ρ as a slow adiabatic variable and the hyperangle α as the fast variable. The eigenvalue $\lambda(\rho) \equiv \nu^2(\rho) - 4$ of the fast hyperangular motion for a fixed ρ serves as the adiabatic potential for the slow hyperradial motion. The eigenvalue is found by solving the Faddeev equation for fixed $\rho \geq \rho_c \equiv 2r_0\sqrt{\mu}$,

$$\Big[-\frac{\partial^2}{\partial\alpha^2} - \nu^2 + U\Big]\psi = -2U\mathcal{R}[\psi]. \qquad (1)$$

Here $\psi(\rho,\alpha)$ is the Faddeev hyperangular component,

$$U(\rho,\alpha) = V(\rho\sin\alpha/\sqrt{\mu})\, m\rho^2/(\hbar^2\mu) \qquad (2)$$

is the rescaled potential, and

$$\mathcal{R}[\psi](\rho,\alpha) \equiv \frac{2}{\sqrt{3}}\int_{|\frac{\pi}{3}-\alpha|}^{\frac{\pi}{2}-|\frac{\pi}{6}-\alpha|} \psi(\rho,\alpha')\,\mathrm{d}\alpha' \qquad (3)$$

is the operator that rotates a Faddeev component into another Jacobi system and projects it onto s-waves. The

total wave-function of the three-body system is $\Psi(\rho,\alpha) = f(\rho)\rho^{-5/2}\,\Phi(\rho,\alpha)$ where

$$\Phi(\rho,\alpha) = \frac{\psi(\rho,\alpha) + 2\mathcal{R}[\psi](\rho,\alpha)}{\sin 2\alpha}. \tag{4}$$

The hyperradial function $f(\rho)$ satisfies the ordinary hyperradial equation [12] with the effective potential

$$V_{\rm eff}(\rho) = \frac{\hbar^2\mu}{m}\Big(\frac{\nu^2-\frac{1}{4}}{\rho^2} - Q\Big), \quad Q = \langle\Phi|\,\frac{\partial^2}{\partial\rho^2}\,|\Phi\rangle\,, \tag{5}$$

where Q is the non-adiabatic term and Φ is normalized to unity for fixed ρ.

We first divide the α-interval $[0;\pi/2]$ into two regions: (I) where $U\neq 0$, and (II) where $U=0$. The regions are separated at $\alpha=\alpha_0$ where $\sin\alpha_0 \equiv \sqrt{\mu}r_0/\rho = \rho_c/(2\rho)$. In region (II) we have the free solution to Eq. (1),

$$\psi^{II}(\alpha) = N(\rho)\sin(\nu\alpha - \nu\frac{\pi}{2}) \tag{6}$$

with the boundary condition, $\psi^{II}(\frac{\pi}{2})=0$ and normalization $N(\rho)$. In region (I), since $\alpha_0 < \pi/6$, Eq. (1) simplifies to

$$\Big[-\frac{\partial^2}{\partial\alpha^2} - \nu^2 + U\Big]\psi^I = -2U\mathcal{R}[\psi^{II}], \tag{7}$$

with the solution $\psi^I = \psi^{Ih} - 2\mathcal{R}[\psi^{II}]$, where ψ^{Ih} and $-2\mathcal{R}[\psi^{II}]$ are homogeneous and inhomogeneous solutions, respectively. ψ^{Ih} is the regular solution to

$$\Big[-\frac{\hbar^2}{m}\frac{\partial^2}{\partial r^2} - \frac{\hbar^2 k_\rho^2}{m} + V_\rho(r)\Big]\psi^{Ih} = 0, \tag{8}$$

$$V_\rho(r) \equiv V(\frac{\rho}{\sqrt{\mu}}\sin(\frac{\sqrt{\mu}}{\rho}r)), \tag{9}$$

where $k_\rho = \sqrt{\mu}\nu/\rho$ and $r = \alpha\rho/\sqrt{\mu}$. When $\alpha\to\alpha_0$,

$$\psi^{Ih} \propto \sin(k_\rho r + \delta_\rho), \tag{10}$$

where the modified phase shift $\delta_\rho(k_\rho)$ arises from the modified two-body potential, V_ρ. The solutions Φ in region (I) and (II) are now matched smoothly, leading to

$$\frac{\partial}{\partial\alpha}\ln\psi^{Ih}\big|_{\alpha_0} = \frac{\partial}{\partial\alpha}\ln\big(\psi^{II} + 2\mathcal{R}[\psi^{II}]\big)\big|_{\alpha_0}. \tag{11}$$

After inserting Eqs. (6) and (10), this equation becomes

$$\frac{\sqrt{\mu}}{\rho}\,\frac{-\nu\cos(\nu\frac{\pi}{2}) + \frac{8}{\sqrt{3}}\sin(\nu\frac{\pi}{6})}{\sin(\nu\frac{\pi}{2})} = k_\rho\cot\delta_\rho(k_\rho), \tag{12}$$

which defines ν as function of ρ. The right-hand-side deviates from the zero-range approximations [5, 10] by using the rigorously defined phase shifts δ_ρ for V_ρ instead of the original phase shifts δ.

Effective range expansion. In the limit $\rho \gg \rho_c$, the ρ-dependent potential, $V_\rho(r)$, approaches $V(r)$, and consequently δ_ρ approaches δ. The ρ-dependent low-energy effective range expansion corresponding to V_ρ is then to second order

$$k_\rho\cot\delta_\rho(k_\rho)\Big|_{k_\rho\to 0} \approx -\frac{1}{a(\rho)} + \frac{R_e(\rho)}{2}k_\rho^2, \tag{13}$$

where $a(\rho)$ and $R_e(\rho)$ are functions of $1/\rho^2$ that converge to a and R_e for $\rho\to\infty$. Up to $1/\rho^2$ in Eq. (13) we get

$$\frac{1}{a(\rho)} \approx \frac{1}{a} + R_V\frac{\mu}{\rho^2}, \quad R_e(\rho)\approx R_e. \tag{14}$$

The model dependent expansion parameter R_V, or "scattering length correction", is found to be

$$R_V = \frac{m}{6\hbar^2}\langle V' r^3\rangle_u = \frac{m}{6\hbar^2}\int_0^{r_0} V'(r)r^3u(r)^2\,\mathrm{d}r, \tag{15}$$

where u is the zero-energy two-body radial wavefunction, asymptotically equal to $1-r/a$. Eq. (12) then becomes

$$\frac{\sqrt{\mu}}{\rho}\,\frac{-\nu\cos(\nu\frac{\pi}{2}) + \frac{8}{\sqrt{3}}\sin(\nu\frac{\pi}{6})}{\sin(\nu\frac{\pi}{2})} = -\frac{1}{a} + \frac{R_e}{2}\frac{\nu^2\mu}{\rho^2} - \frac{R_V\mu}{\rho^2}. \tag{16}$$

This equation without the last two finite range terms has the well-known purely imaginary solution $\nu_0 = 1.00624i$, or $\lambda_0 = -5.0125$, for $\rho/\sqrt{\mu} \ll |a|$. This solution gives $V_{\rm eff} \propto -1/\rho^2$ which is the basis of Efimov physics. The R_e-term was included in [5, 7], but not the model dependent R_V-term. The latter term makes the finite-range corrections to the zero-range adiabatic eigenvalues explicitly non-universal. The last two terms in Eq. (16) restrict the solution λ_0 to the region $|R_0| \ll \rho/\sqrt{\mu} \ll |a|$, where

$$R_0 = \frac{R_e}{2}\nu_0^2 - R_V, \tag{17}$$

as seen in Fig. 1 where the lowest solution to Eq. (16) is shown for different parameter choices. Thus, naively one would think that the lower limit for Efimov physics is determined by the model dependent length $|R_0|$. However, we will show later that Q restores universality and recovers the model independent effective range, R_e.

First, to illustrate the necessity of both $1/\rho^2$-terms in Eq. (16) we consider a large negative effective range corresponding to a narrow Feshbach resonance [9]. To model the large $|R_e|$ we pick an attractive potential with barrier

$$V(r) = D\,\mathrm{sech}^2\Big(\chi\frac{r}{r_0}\Big) + B\exp\Big(-2(\chi\frac{r}{r_0} - 2)^2\Big), \tag{18}$$

where $D=-138.27$, $B=128.49$ in units of $\hbar^2/(mr_0^2)$, and $\chi=4.6667$. The potential is negligible outside the range r_0. The low-energy parameters are $a=556.88$, $R_e=-142.86$, $R_V=73.031$, and $R_0=-0.71$ in units of

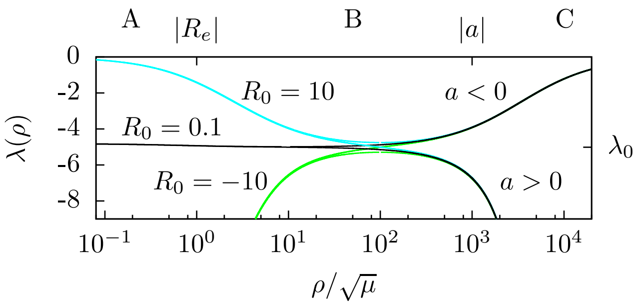

FIG. 1: (color online) Adiabatic eigenvalues $\lambda(\rho)$ from Eq. (16) as function of hyperradius ρ, for large scattering length a and negative R_e. Different values of the model dependent length R_0 are used, showing that the universal solution λ_0 exists in the region $|R_0| \ll \rho/\sqrt{\mu} \ll |a|$. Lengths are in units of $|R_e|$.

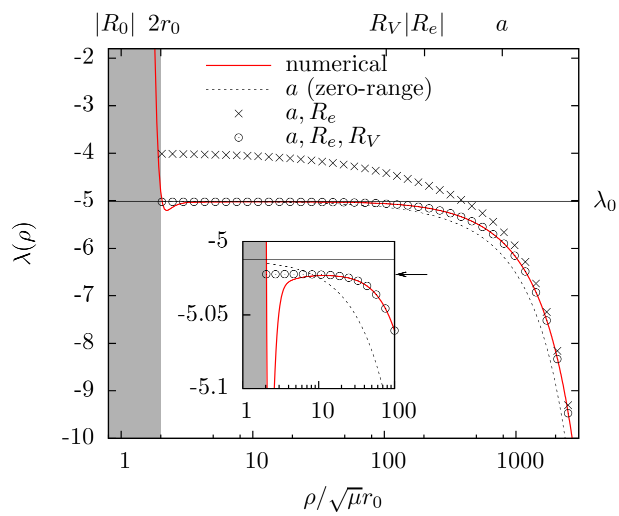

FIG. 2: (color online) Exact numerical adiabatic eigenvalues $\lambda(\rho)$ for a potential with barrier, Eq. (18) (solid red line), compared to solutions of the eigenvalue equation, Eq. (16). The zero-range model (dotted line) includes only a. Crosses include a, R_e-terms and circles include a, R_e, R_V-terms. The inset shows details around λ_0. The arrow indicates the effect of the correction $\lambda_0 - 2R_0/R_e$.

r_0. In Fig. 2 we compare $\lambda(\rho)$ obtained by exact numerical solution of the Schrödinger equation [11] containing the interaction Eq. (18) with the solution of Eq. (16). In the zero-range model (including only $1/a$), the $-\rho^2$ divergence for large ρ is below the numerical solution. At small distances, λ approaches λ_0, above the numerical solution. Inclusion of the R_e-term, as in [5, 7], provides a better large-distance behavior (since the dimer binding energy is corrected), but overshoots dramatically for $\rho/\sqrt{\mu} \lesssim a$ by approaching $\lambda = -4$. Including consistently both R_e- and R_V-terms leads to complete numerical agreement with the exact numerical solution except for very small ρ-values where higher order terms are needed in Eq. (16).

Non-adiabatic corrections. We shall show that the non-adiabatic term restores model independence and recovers $|R_e|$ as the limit for the region of Efimov physics. For simplicity we only consider the limit $|a| = \infty$ and assume $|R_0| \ll |R_e|$. We first consider $\rho/\sqrt{\mu} \ll |R_e|$ (region A in Fig. 1). Expansion of Eq. (16) to first order in $(\nu - \nu_0)$ gives a small constant correction

$$\nu = \nu_0 - \frac{R_0}{\nu_0 R_e}\Big(1 + O(\frac{\rho}{R_e})\Big). \tag{19}$$

This correction is marked by the arrow in Fig. 2 (it is out of the range of Fig. 1). This gives

$$V_{\text{eff}}(\rho) = \frac{\hbar^2\mu}{m}\Big(\frac{\nu_0^2 - 1/4 - 2R_0/R_e}{\rho^2} - Q\Big). \tag{20}$$

To evaluate Q we note that a large negative effective range (for $|a| = \infty$) implies that the two-body wavefunction u is localized mainly inside the potential range. Then the angular three-body wavefunction Φ can be approximated by $u/\sin(2\alpha)$. The result is $Q = c/\rho^2$, where $c \simeq -5/4$ as confirmed numerically. This term cancels the main $1/\rho^2$-part in Eq. (20) and hence prohibits Efimov physics for $\rho/\sqrt{\mu} \ll |R_e|$. The intuitive reason is that the two-body wavefunction is essentially zero outside the potential, despite the large scattering length, and hence three particles can not interact at large distances.

When $\rho/\sqrt{\mu} \gg |R_e|$ (region B in Fig. 1) we find

$$\nu = \nu_0 + \nu_0 c_0 \frac{R_0\sqrt{\mu}}{\rho}\Big(1 + O(\frac{R_e}{\rho})\Big), \tag{21}$$

$$c_0 = \frac{\sin(\nu_0\frac{\pi}{2})/\nu_0}{\frac{4\pi}{3\sqrt{3}}\cos(\nu_0\frac{\pi}{6}) - \cos(\nu_0\frac{\pi}{2}) + \nu_0\frac{\pi}{2}\sin(\nu_0\frac{\pi}{2})}, \tag{22}$$

or $c_0 \simeq -0.671$. This gives

$$V_{\text{eff}}(\rho) = \frac{\hbar^2\mu}{m}\Big(\frac{\nu_0^2 - 1/4}{\rho^2} + \frac{c_0\nu_0^2\sqrt{\mu}}{\rho^3}\left(R_e\nu_0^2 - 2R_V\right) - Q\Big). \tag{23}$$

The $1/\rho^3$ dependence of the correction to the Efimov potential $1/\rho^2$ was expected [6]. The model independent term proportional to R_e/ρ^3 was recently calculated in [5]. However, we also get a model dependent term R_V/ρ^3 which is of the same order. Q generally receives contributions both from distances inside and outside the finite-range potential. Zero-range models only have the external part of the wavefunction, which depends on ρ only though the eigenvalue $\nu(\rho)$. The zero-range result for Q is then

$$Q_{\text{ZR}} = M_0(\frac{\partial\nu}{\partial\rho})^2 = M_0 c_0^2\nu_0^2\frac{R_0^2\mu}{\rho^4}, \tag{24}$$

where $M_0 = \langle\Phi|\partial^2\Phi/\partial\nu^2\rangle|_{\nu=\nu_0}$. This fourth order correction can be neglected in Eq. (23), as was done in [5]. However, the internal part of the wavefunction contributes to

order $1/\rho^3$. To estimate this $1/\rho^3$-term we take the analytically solvable finite square well potential of range r_0 and $|a| = \infty$. This fixes $R_e = r_0$ and $R_V = n^2\pi^2 r_0/24$ where n is the number of bound states (including the zero-energy state). We find

$$Q_{\rm box} = c_0\nu_0^2(\frac{R_e}{2} - 2R_V)\frac{\sqrt{\mu}}{\rho^3}, \quad (25)$$

neglecting $1/\rho^4$-terms. The model dependent R_V-terms in Eqs. (23) and (25) cancel exactly, giving

$$V_{\rm eff}^{\rm box}(\rho) = \frac{\hbar^2\mu}{m}\Big(\frac{\nu_0^2 - 1/4}{\rho^2} + c_0\nu_0^2(\nu_0^2 - \frac{1}{2})\frac{\sqrt{\mu}R_e}{\rho^3}\Big). \quad (26)$$

So the effective potential receives a R_e/ρ^3 correction where the model dependent coefficient is different from zero-range models [5] because of the inclusion of Q. We also expect the R_V-terms to cancel for general potentials. In conclusion, the Efimov effect persists for $\rho/\sqrt{\mu} \gg |R_e|$.

Atom-dimer potential. We have seen that model dependent corrections to λ_0 are cancelled by equivalent terms in Q. A similar effect occurs for the atom-dimer channel potential. Suppose the binding energy is $B_D = \hbar^2 k_D^2/m$ with corresponding wave number $k_D > 0$. Then $\nu = ik_D\rho/\sqrt{\mu}$ is an asymptotic solution to Eq. (12) and λ diverges as $-\rho^2$ corresponding to a bound dimer and a free particle. For this solution, the effective range expansion Eq. (13) does not hold, since asymptotically $k_\rho \to ik_D$ is finite. Instead Eq. (8) reduces to the radial two-body equation, with a normalized bound state s-wave function $u_D(r)$. Treating $V_\rho - V \propto 1/\rho^2$ as a perturbation gives the correction

$$\frac{\lambda+4}{\rho^2} = -\frac{k_D^2}{\mu} - \int_0^\infty r^3 u_D^2 \frac{mV'(r)}{6\hbar^2}\,\mathrm{d}r\frac{1}{\rho^2} + O(\frac{1}{\rho^4}). \quad (27)$$

Since $\mathcal{R}[\psi]$ is exponentially small for the atom-dimer solution, Q can be computed using the unperturbed wavefunction $\psi = \sqrt{\rho}u_D(\alpha\rho/\sqrt{\mu})$, giving

$$Q = -\frac{1}{4\rho^2} + \int_0^\infty u_D(ru_D' + r^2u_D'')\,\mathrm{d}r\frac{1}{\rho^2} + O(\frac{1}{\rho^4}). \quad (28)$$

By using the two-body radial equation and partial integration the two integrals in Eqs. (27) and (28) cancel. Thus the $1/\rho^2$-terms in the effective potential Eq. (5) cancel exactly, giving $V_{\rm eff}(\rho) = -B_D$ up to order $1/\rho^4$. Thus $V_{\rm eff}$ only depends on R_e through B_D.

Effective range for Feshbach resonances. The effective range near a Feshbach resonance has been estimated using a coupled-channels zero-range model [9], as

$$R_e = -2(\Delta B\, m\, \Delta\mu\, a_{bg})^{-1}, \quad (29)$$

where ΔB is the magnetic field width, $\Delta\mu$ is the magnetic moment difference between the channels, and a_{bg} is the background scattering length. As an example we take the alkali atoms ^{39}K with the very narrow Feshbach resonance at $B = 825$G having parameters $\Delta B = -32$mG, $\Delta\mu = -3.92\mu_B$, and $a_{bg} = -36a_0$ [13]. This gives the large effective range $R_e = -2.93\times10^4 a_0$. For ^{39}K, r_0 is of the order of the van der Waals length $l_{\rm vdW} = 1.29\times10^2 a_0$ [4]. Since $|R_e| \gg r_0$, $|R_e|$ determines the lower limit for Efimov physics and corrections to the universal regime are of order R_e/a (not $l_{\rm vdW}/a$). Thus, the window for universal physics is reduced.

Summary and Conclusions. We consider a three-body system of identical bosons with large scattering length modelling a Feshbach resonance. The Efimov physics occurring in this "universal regime" is customarily accounted for by zero-range models. We use the adiabatic hyperspherical approximation and derive rigorously a transcendental equation to determine the asymptotic adiabatic potential for a general finite-range potential. We solve this equation for large scattering length, investigate finite range effects, and compare with exact numerical results.

Inclusion of the effective range correction to the adiabatic potential is insufficient in general. Crucial corrections of the same order must also be included from both the scattering length and the non-adiabatic term. These two contributions may separately be large but they tend to cancel each other. Accurate results in zero-range models must account for these new corrections. In conclusion, the window for Efimov physics is precisely open between the effective range (not the potential range) and the scattering length.

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